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NEWS 25	JUN 06	EPFULL enhanced with 260,000 English abstracts
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NEWS 27	JUN 13	USPATFULL and USPAT2 updated with 11-character patent numbers for U.S. applications
NEWS 28	JUN 19	CAS REGISTRY includes selected substances from web-based collections
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=> s dinitrotoluene (5w) nitrocresol (l) prepare
4495 DINITROTOLUENE
285 DINITROTOLUENES

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          4576 DINITROTOLUENE
                 (DINITROTOLUENE OR DINITROTOLUENES)
           296 NITROCRESOL
            83 NITROCRESOLS
           349 NITROCRESOL
                 (NITROCRESOL OR NITROCRESOLS)
         11228 PREPARE
          1991 PREPARES
         13175 PREPARE
                 (PREPARE OR PREPARES)
        139238 PREP
          2387 PREPS
        141401 PREP
                 (PREP OR PREPS)
        153043 PREPARE
                 (PREPARE OR PREP)
L1           0 DINITROTOLUENE (5W) NITROCRESOL (L) PREPARE

=> s dinitrotoluene (L) nitrocresol
          4495 DINITROTOLUENE
           285 DINITROTOLUENES
          4576 DINITROTOLUENE
                 (DINITROTOLUENE OR DINITROTOLUENES)
           296 NITROCRESOL
            83 NITROCRESOLS
           349 NITROCRESOL
                 (NITROCRESOL OR NITROCRESOLS)
L2           12 DINITROTOLUENE (L) NITROCRESOL

=> d l2 1-6 ibib abs

L2   ANSWER 1 OF 12  CAPLUS  COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER:        2005:424704  CAPLUS
DOCUMENT NUMBER:         143:128881
TITLE:                   Protein engineering of the archetypal nitroarene
                         dioxygenase of Ralstonia sp. strain U2 for activity on
                         aminonitrotoluenes and dinitrotoluenes through
                         alpha-subunit residues leucine 225, phenylalanine 350,
                         and glycine 407
AUTHOR(S):               Keenan, Brendan G.; Leungsakul, Thammajun; Smets,
                         Barth F.; Mori, Masa-aki; Henderson, David E.; Wood,
                         Thomas K.
CORPORATE SOURCE:        Departments of Chemical Engineering and Molecular and
                         Cell Biology, University of Connecticut, Storrs, CT,
                         06269-3222, USA
SOURCE:                  Journal of Bacteriology (2005), 187(10), 3302-3310
                         CODEN: JOBAAY; ISSN: 0021-9193
PUBLISHER:               American Society for Microbiology
DOCUMENT TYPE:           Journal
LANGUAGE:                English
AB   Naphthalene dioxygenase (NDO) from Ralstonia sp. strain U2 has not been
     reported to oxidize nitroarom. compds.  Here, saturation mutagenesis of NDO at
     position F350 of the α-subunit (NagAc) created variant F350T that
     produced 3-methyl-4-nitrocatechol from 2,6-dinitrotoluene
     (26DNT), that released nitrite from 2,3-dinitrotoluene (23DNT)
     sixfold faster than wild-type NDO, and that produced 3-amino-4-methyl-5-
     nitrocatechol and 2-amino-4,6-dinitrobenzyl alc. from 2-amino-4,6-
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dinitrotoluene (2A46DNT) (wild-type NDO has no detectable activity on 26DNT and 2A46DNT). DNA shuffling identified the beneficial NagAc mutation G407S, which when combined with the F350T substitution, increased the rate of NDO oxidation of 26DNT, 23DNT, and 2A46DNT threefold relative to variant F350T. DNA shuffling of NDO nagAcAd also generated the NagAc variant G50S/L225R/A269T with an increased rate of 4-amino-2-nitrotoluene (4A2NT; reduction product of 2,4-dinitrotoluene) oxidation; from 4A2NT, this variant produced both the previously uncharacterized oxidation product 4-amino-2-nitrocresol (enhanced 11-fold relative to wild-type NDO) as well as 4-amino-2-nitrobenzyl alc. (4A2NBA; wild-type NDO does not generate this product). G50S/L225R/A269T also had increased nitrite release from 23DNT (14-fold relative to wild-type NDO) and generated 2,3-dinitrobenzyl alc. (23DNBA) fourfold relative to wild-type NDO. The importance of position L225 for catalysis was confirmed through saturation mutagenesis; relative to wild-type NDO, NDO variant L225R had 12-fold faster generation of 4-amino-2-nitrocresol and production of 4A2NBA from 4A2NT as well as 24-fold faster generation of nitrite and 15-fold faster generation of 23DNBA from 23DNT. Hence, random mutagenesis discovered two new residues, G407 and L225, that influence the regiospecificity of Rieske non-heme-iron dioxygenases.

REFERENCE COUNT: 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L2 ANSWER 2 OF 12 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:371207 CAPLUS
DOCUMENT NUMBER: 142:413314
TITLE: Extraction of nitrocresols from wastewater produced in the manufacture of mononitrotoluene and use of the extract
INVENTOR(S): Buettner, Johannes; Allardt, Holger; Tonder, Reinhard; Reetz, Reiner; Reichelt, Michael
PATENT ASSIGNEE(S): BASF Aktiengesellschaft, Germany
SOURCE: PCT Int. Appl., 13 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005037766	A1	20050428	WO 2004-EP10497	20040918
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
DE 10345601	A1	20050512	DE 2003-10345601	20030929
EP 1670745	A1	20060621	EP 2004-765388	20040918
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				

CN 1860095	A	20061108	CN 2004-80028163		20040918
JP 2007506799	T	20070322	JP 2006-529997		20040918
US 20070043244	A1	20070222	US 2006-573020		20060322
PRIORITY APPLN. INFO.:			DE 2003-10345601	A	20030929
			WO 2004-EP10497	W	20040918

AB The alkaline wastewater produced in the manufacture of O2NC6H4Me is acidified with acids, e.g., H2SO4 and/or HNO3 to pH ≤3, and the nitrocresols are extracted preferably with PhMe, o-, m- or p-O2NC6H4Me, or their mixts. The extract containing nitrocresols is used as a feedstock for manufacture of dinitrotoluene.

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L2 ANSWER 3 OF 12 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:1093 CAPLUS
DOCUMENT NUMBER: 142:96315
TITLE: Phase-separation process for working up secondary components in the preparation of dinitrotoluene by the nitration of toluene
INVENTOR(S): Munnig, Jurgen; Wastian, Dietmar; Lorenz, Wolfgang; Keggenhoff, Berthold
PATENT ASSIGNEE(S): Bayer Materialscience AG, Germany
SOURCE: U.S. Pat. Appl. Publ., 4 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
US 20040267062	A1	20041230	US 2004-878079		20040628
US 6953869	B2	20051011			
DE 10329303	A1	20050203	DE 2003-10329303		20030630
EP 1493730	A1	20050105	EP 2004-14228		20040617
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR					
KR 2005002619	A	20050107	KR 2004-49537		20040629
CN 1576240	A	20050209	CN 2004-10063300		20040629
JP 2005023076	A	20050127	JP 2004-194526		20040630
PRIORITY APPLN. INFO.:			DE 2003-10329303	A	20030630

AB A process is described for working up organic secondary components which are formed in the one-stage or two-stage nitration of toluene to dinitrotoluene, the organic secondary components are present in the acidic and alkaline waste water from the dinitrotoluene-washing step and in the aqueous distillate from the sulfuric acid concentration step, together with small amts. of nitrotoluene and dinitrotoluene. This process comprises: (A) combining the acidic and alkaline waste waters from the washing step and the aqueous distillate from the sulfuric acid-concentration step such that the resulting mixture has a pH <5; (B) separating the aqueous and organic phases which form by phase separation; and (C) recycling the organic phase from step (B) into the nitration process.

REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L2 ANSWER 4 OF 12 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1999:783737 CAPLUS
DOCUMENT NUMBER: 132:6012
TITLE: Dilute acid oxidation of dinitrotoluene alkaline wash water
INVENTOR(S): Van Court, Carr Richard; Simpson, Mark Shedric
PATENT ASSIGNEE(S): Air Products and Chemicals, Inc., USA
SOURCE: Eur. Pat. Appl., 7 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 962446	A1	19991208	EP 1998-109789	19980528
EP 962446	B1	20010801		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
CN 1203904	A	19990106	CN 1998-108262	19980501
PRIORITY APPLN. INFO.:			CN 1998-108262 A	19980501
			US 1997-848933 A	19970501

AB Nitrocresols in a crude aqueous alkaline dinitrotoluene wash stream are removed using a dilute oxidizing acid such as nitric acid or sulfuric acid, heated to 130 to 180°C for a period of time required to reduce the nitrocresols to a level at which it does not precipitate from the mixed acidic wash stream at temps. above about 60°C. Removal of the remaining nitrocresols can be achieved by conventional methods such as carbon adsorption or activated sludge biotreatment. For comparison, dilute oxidizing acids are also used to treat dinitrophenols in a crude aqueous mononitrobenzene wash stream. Both 2,6-dinitrophenol and 2,4-dinitrophenol were removed, but the process was shown not to involve oxidation and picric acid was produced.
REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L2 ANSWER 5 OF 12 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1998:392206 CAPLUS
DOCUMENT NUMBER: 129:71603
ORIGINAL REFERENCE NO.: 129:14755a,14758a
TITLE: Dilute acid oxidation of dinitrotoluene alkaline wash water
INVENTOR(S): Van Court Carr, Richard; Simpson, Mark Shedrick
PATENT ASSIGNEE(S): Air Products and Chemicals, Inc., USA
SOURCE: U.S., 4 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5762802	A	19980609	US 1997-848933	19970501

BR 9801469 A 20000208 BR 1998-1469 19980428
CN 1203904 A 19990106 CN 1998-108262 19980501
PRIORITY APPLN. INFO.: US 1997-848933 A 19970501
AB A process for removing nitrocresols in a crude aqueous alkaline dinitrotoluene wash stream derived by nitration of toluene using a mixed acid technique followed by treatment with aqueous alkaline material in which the crude aqueous alkaline dinitrotoluene wash stream is mixed with a dilute oxidizing acid such as nitric acid, heated to 130° to 180°. for a period of time required to reduce the nitrocresols to a level at which it does not precipitate from the mixed acidic wash stream at temps. above about 60°., and removing the remaining nitrocresols by conventional methods such as adsorption or activated sludge biotreatment.
REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L2 ANSWER 6 OF 12 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1987:611289 CAPLUS
DOCUMENT NUMBER: 107:211289
ORIGINAL REFERENCE NO.: 107:33731a,33734a
TITLE: Spectrophotometric determination of dinitrocresol in industrial dinitrotoluene
AUTHOR(S): Wang, Zhaoming; Fu, Ruonong
CORPORATE SOURCE: Dep. Chem. Eng., Beijing Ind. Coll., Beijing, Peop. Rep. China
SOURCE: Fenxi Huaxue (1987), 15(7), 670
CODEN: FHHHDT; ISSN: 0253-3820
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
AB Dinitrocresol in industrial dinitrotoluene was extracted with dilute KOH solution, followed by addition of a known amount of standard 2-methyl-3,5-dinitrophenol or 4-methyl-3,5-dinitrophenol. The dinitrocresol was determined by measuring the absorbance at 436 nm vs. the same solution which was acidified with 6M HCl. Beer's law was obeyed for dinitrocresol at 2.5 + 10-3 - 2.5 + 10-2 mg/mL. The relative standard deviation was <1% in the determination of 0.002% dinitrocresol in dinitrotoluene. The recovery of dinitrocresol was >95%.

=> d l2 7-12 ibib abs

L2 ANSWER 7 OF 12 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1986:539142 CAPLUS
DOCUMENT NUMBER: 105:139142
ORIGINAL REFERENCE NO.: 105:22363a,22366a
TITLE: Removal of nitrocresols from dinitrotoluene waste streams using Fenton's reagent
INVENTOR(S): Carr, Richard V. C.; Martin, Carl J.; Gonzalez, Roland; Albanese, Thomas A.
PATENT ASSIGNEE(S): Air Products and Chemicals, Inc., USA
SOURCE: U.S., 4 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent

LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4604214	A	19860805	US 1985-766849	19850816

PRIORITY APPLN. INFO.: US 1985-766849 19850816
OTHER SOURCE(S): MARPAT 105:139142
AB Nitrocresols and picric acid are removed from wastewaters from nitroaroms. production, e.g. dinitrotoluene, by washing the crude product with alkaline medium, e.g. Na2CO3, NH4OH, NaOH, NaHCO3, or KOH, until concentration of the water-soluble trinitrocresol and picric acid salts is sufficiently high, reducing the pH of the wastewater to 3-4 using aqueous acid, e.g., H2SO4 or HNO3, and then adding H2O2 and Fe2+ to oxidize the trinitrocresol to carboxylic acid, HNO3, and CO2. The Fe2+ may be FeSO4.

L2 ANSWER 8 OF 12 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1986:465887 CAPLUS
DOCUMENT NUMBER: 105:65887
ORIGINAL REFERENCE NO.: 105:10655a,10658a
TITLE: Precipitative removal of nitrocresols from dinitrotoluene waste streams
INVENTOR(S): Carr, Richard V. C.; Sawicki, John E.; Toseland, Bernard A.
PATENT ASSIGNEE(S): Air Products and Chemicals, Inc., USA
SOURCE: U.S., 4 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4597875	A	19860701	US 1985-731424	19850507

PRIORITY APPLN. INFO.: US 1985-731424 19850507
OTHER SOURCE(S): MARPAT 105:65887
AB An alkaline wash water containing water soluble nitrocresols and picric acid from the manufacture of dinitrotoluene is recycled through the wash process and then treated with aqueous acid to precipitate the orgs. The orgs. are removed and incinerated. Thus, wash water that contained 1.13 weight% trinitrocresols was adjusted to pH 1 with H2SO4. The liquid precipitate contained 88% of the orgs. and was removed and incinerated.

L2 ANSWER 9 OF 12 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1986:38945 CAPLUS
DOCUMENT NUMBER: 104:38945
ORIGINAL REFERENCE NO.: 104:6310h,6311a
TITLE: A continuous stirred tank reactor investigation of the gas-phase reaction of hydroxyl radicals and toluene
AUTHOR(S): Gery, Michael W.; Fox, Donald L.; Jeffries, Harvey E.; Stockburger, Leonard; Weathers, Walter S.
CORPORATE SOURCE: Sch. Public Health, Univ. North Carolina, Chapel Hill, NC, 27514, USA

SOURCE: International Journal of Chemical Kinetics (1985), 17(9), 931-55
CODEN: IJCKBO; ISSN: 0538-8066
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A continuous stirred tank reactor (CSTR) was used to study the gas-phase reaction between OH radicals and PhMe [108-88-3]. The OH radicals were generated by the in-situ photolysis of HNO2. Flow reactor operation at steady-state conditions with a residence time of 20 min allowed investigation of primary and very rapid secondary reactions. CSTR and batch reactor expts. were also performed with selected products. Both gas-phase and aerosol products were identified by chromatog. and mass spectroscopy, with total product yields between 55 and 75% of reacted C. PhMe reaction products included cresols, nitrocresols, nitrotoluenes, 3,5-dinitrotoluene [618-85-9], benzaldehyde [100-52-7], benzyl nitrate [15285-42-4], methyl-p-benzoquinone [553-97-9], glyoxal [107-22-2], methylglyoxal [78-98-8], HCHO [50-00-0], peroxyacetyl nitrate [2278-22-0], CO, and nitrophenols. The fraction of abstraction of Me H atoms by OH radicals was calculated to be 0.13 ± 0.04. The ratio of reaction rate consts. for nitrotoluene vs. cresol formation from the HO adduct was calculated to be .apprx.3.3 + 104. Also, the ratio of cresol formation vs. O2 addition to the HO adduct was estimated to be ≥0.5 for atmospheric conditions. Comparisons of these measurements with previous values and the implications with respect to photochem. kinetic modeling of the atmospheric are discussed.

L2 ANSWER 10 OF 12 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1984:576631 CAPLUS
DOCUMENT NUMBER: 101:176631
ORIGINAL REFERENCE NO.: 101:26656h,26657a
TITLE: Atmospheric reactions of o-cresol: gas phase and aerosol products
AUTHOR(S): Grosjean, Daniel
CORPORATE SOURCE: Environ. Res. and Technol., Inc., Westlake Village, CA, 91361, USA
SOURCE: Atmospheric Environment (1967-1989) (1984), 18(8), 1641-52
CODEN: ATENBP; ISSN: 0004-6981
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Photochem- oxidation of o-cresol [95-48-7] (0.5-1.u ppm) and NOx (0.12-0.66 ppm) in air yielded the following gas-phase products: pyruvic acid [127-17-3], AcH [75-07-0], HCHO [50-00-0], peroxyacetylnitrate [2278-22-0], nitrocresol [12167-20-3] and trace levels of HNO3 and methyl nitrate [598-58-3]. Particulate phase products included 2-hydroxy-3-nitrotoluene [13073-29-5], 2-hydroxy-5-nitrotoluene [99-53-6], 2-hydroxy-3,5-dinitrotoluene [534-52-1] and, tentatively, several hydroxy-nitrocresol isomers. Yields of gas-phase products (0.8% for pyruvic acid, 5-11% for the sum of the aromatic ring fragmentation products) and of aerosol products (5-19% on a C basis, with particulate C formation rates of 30-80 μg/m3-h) are discussed in terms of photochem. reaction pathways. From 60 to 89% of the initial NOx was consumed in these reactions, and a significant fraction of the reacted NOx could be accounted for as particulate nitroarom. products.

L2 ANSWER 11 OF 12 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1916:4978 CAPLUS

DOCUMENT NUMBER: 10:4978
ORIGINAL REFERENCE NO.: 10:967f-i,968a-d
TITLE: Trinitrotoluene
AUTHOR(S): Copisarow, M.
SOURCE: Chemical News and Journal of Industrial Science (1915), 112, 247-8
CODEN: CHNWAY
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB cf. following abstract. Six isomers of trinitrotoluene are known: α-, 2, 4,6,m. 80.8°; β-,2,3,4, m. 112°; γ-,2,4,5,m. 104°; δ-,3,4,5,m.137-5°; ε,2,3,5,m. 97.2°;ζ,2,3,6,m. 79-5°. Com. trinitrotoluene, while principally the α-form, is accompanied by other modifications, produced from m-nitrotoluene, which constitute about 4.5% of the com. mononitrotoluene. All of the isomers of trinitrotoluene are of practically the same value as explosives. They may be distinguished by acetone and NH3 with which the a-form gives deep red, β-form. greenish yellow, γ-form blue, ε-form rose-red and the ζ-form orange-red. The manufacture of trinitotoluene is usually carried out in 2 or 3 stages, the concentration of acids being gradually increased, and although by itself a simple process, numerous chemical and technical difficulties are met with when the manufacture is conducted on a large scale. Chief among these is the presence in the product of inorganic impurities derived from Pb compds. in the acids or from the action of the acids on the apparatus in which the nitration is carried out, and of organic intermediate compds. and by-products due to imperfect stirring, to concentration and ratio of acid and to duration and temperature of reaction. A check on the operation may be found in the appearance and analysis of the spent acid which varies in color from yellowish to dark brown, the color being the darker the less the nitric and the more the sulfonic acids, as well as organic matter, present. The mineral matter present during the process may act either as a catalyst or a chemical reagent. When the mineral acids act upon the metal parts of the apparatus H may be set free and it may reduce some of the nitro compds. Under the working conditions amino groups may be diazotized yielding cresols and nitrocresols whose salts are highly sensitive explosives and thus there may be obtained as by-products: (I) trinitrobenzoic acid, and even tetranitromethane, owing to oxidation in case of overheating or pressure. The intense odor of the latter is sometimes observed in the factories, but the former, owing to its solubility, generally escapes detection; (2) phenolic compds., like cresols, owing to the reduction of some of the nitro compds.; (3) sulfonic acids, when the quantity of nitric in the mixed acid is below the minimum. In the process of manufacture of trinitrotoluene the following must be observed: (1) The amount of HNO3 to be used must exceed at least by 1/2 mol. the quantity theoretically required for the carrying out of the nitration to a certain stage. (2) The extent of nitration should be regulated more by the concentration of the acids, temperature, and duration of reaction than by the actual quantity of HNO3 present. (3) The reaction product should not be kept in contact with the spent acid longer than is really unavoidable. (4) The concentration of acid and material of plant should be such as to reduce their action on one another to a minimum. (5) The starting materials (toluene and acids) must be pure. The residue from the mother-liquors consists of a complex mixture of various di- and trinitrotoluenes. By nitrating this with a mixed acid containing only 15% of HNO3 a "liquid

trinitrotoluene" is obtained, which has considerable power, and has the property of gelatinizing collodion cotton, as nitroglycerin does. It is used in the manufacture of gelatinized explosives. It contains 16.6 to 17.2% of N, whereas pure trinitrotoluene contains 18.5% and dinitrotoluene 15.4%. Other details of importance to manufacturers and users of trinitrotoluene are set forth.

L2 ANSWER 12 OF 12 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1906:40356 CAPLUS
DOCUMENT NUMBER: 0:40356
TITLE: On orcinol and some of the other dihydroxytoluenes
AUTHOR(S): Nevile, R. H. C.; Winther, A.
SOURCE: Journal of the Chemical Society, Transactions (1882), 41, 415-428
From: J. Am. Chem. Soc. 5(4), 61-2 1883
CODEN: JCHTA3; ISSN: 0368-1645
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB Believing that Orcinol was a dihydroxytoluene, the authors undertook this investigation. Taking dinitroparatoluene 1:3:5 made from dinitropartoluidine, it was dissolved in alcohol and treated with ammonium sulphide. Water was added and the precipitate dissolved in hydrochloric acid and reprecipitated with ammonia. By further purification thick needles of nitrotoluidine were obtained melting at 98°-98°.4. The yield was 50 percent of the dinitrotoluene used. By treating with sulphuric acid the sulphate was obtained; which by further treatment with potassic nitrite gave nitrocresol as a brown oil, which by purification with ether gave yellow needles of nitrocresol. The nitrocresol was treated with tin and hydrochloric acid; after removing the tin, the solution was evaporated, and the crystals obtained washed with ether to remove unreduced nitrocresol. From this chloride dihydroxytoluene is obtained by treating with sulphuric acid and potassic nitrite. The resulting oil purified by distillation and crystallizing from benzene and chloroform, gives from the first needles or prisms and from the latter white leaves. After 14 days over sulphuric acid it melts at 106°-108°; which by analysis proves to be orcinol C6H3,CH3, (OH)2 1:3:5. The authors have also succeeded in making orcinol from metabromo-toluene-metasulphonic acid; toluene-meta-disulphonic acid; metabromo-metatoluidine; metadibromotoluene. During this research the authors have also obtained the dihydroxytoluene 1:2:4, starting with orthonitro-paratoluidine. This latter was converted in sulphate, treated with potassic nitrite and converted into nitrocresol. This nitrocresol was treated with tin and hydrochloric acid to obtain amido-cresol. The chloride of amido-cresol thus obtained by treatment with sulphuric acid and potassic nitrite and the dihydroxytoluene obtained as an oil, which afterward crystallized, and by sublimation and crystallization gave a melting point of 104°-105°. The author also prepared dihydroxytoluene 1:2:5 from meta-nitro-orthotoluidine following nearly the same process as in above case. The dihydroxytoluene 1:2:5 obtained is in white leaves melting at 124°-125° and freely soluble in alcohol, ether or water. An investigation of the dihydroxytoluene 1:3:4 was also made by the authors starting with metanitro-paratoluidine, following the method above used by preparing the diazo compound, but was unsatisfactory. The method of Wagner (Ber. 1874, 537) was used, and by slight modification with success. The paper is a very lengthy one and filled with most interesting details in manipulation of the methods used.

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=> d his

     (FILE 'HOME' ENTERED AT 15:36:46 ON 26 JUN 2008)

     FILE 'CAPLUS' ENTERED AT 15:37:08 ON 26 JUN 2008
L1             0 S DINITROTOLUENE (5W) NITROCRESOL (L) PREPARE
L2            12 S DINITROTOLUENE (L) NITROCRESOL

=> log off
ALL L# QUERIES AND ANSWER SETS ARE DELETED AT LOGOFF
LOGOFF? (Y)/N/HOLD:y
STN INTERNATIONAL LOGOFF AT 15:41:19 ON 26 JUN 2008
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